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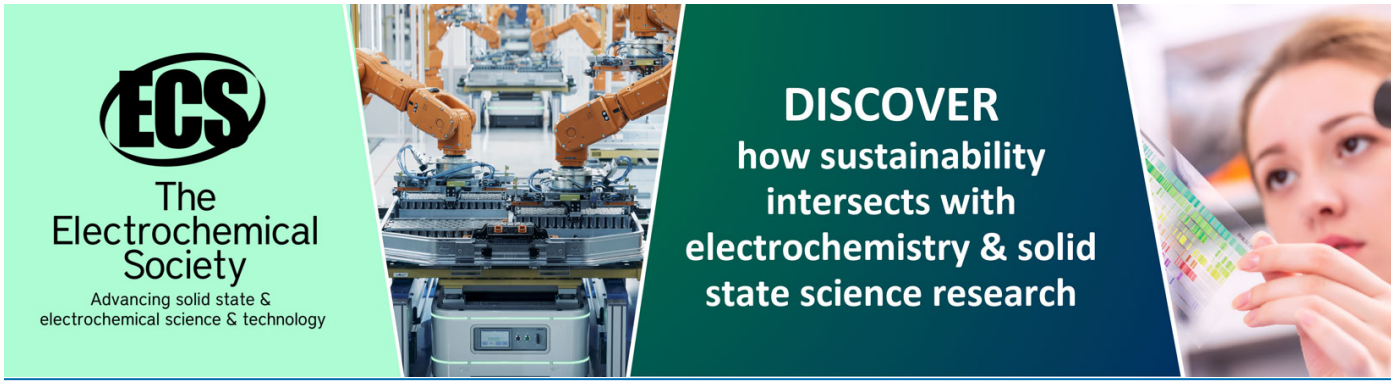

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Computational technology of multiscale modeling the gas flows in microchannels

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Abstract. The work is devoted to modeling the gas mixture flows in engineering microchannels under conditions of many scales of computational domain. The computational technology of using the multiscale approach combining macro - and microscopic models is presented. At macrolevel the nature of the flow and the external influence on it are considered. As a model the system of quasigasdynamic equations is selected. At microlevel the correction of gasdynamic parameters and the determination of boundary conditions are made. As a numerical model the Newton's equations and the molecular dynamics method are selected. Different algorithm types used for implementation of multiscale modeling are considered. The results of the model problems for separate stages are given.

1. Introduction

The modern computer technology makes it possible to simulate very complex systems and processes. Now the research of complex gasdynamic processes in technical micro- and nanosystems which are applied within implementation of nanotechnologies in the industry is very relevant. The paper deals with the process of gas mixture flows in the microchannels of technical systems.

The purpose of gas flows simulation tasks is determination of the optimal flow mode taking into account the geometry of installation, the properties of the gas medium and the solid wall materials. Also the fact should be taken into account that the modern technical systems can have complex multicomponent and multichannel structure. The diameters of the channels can vary from nanometers to millimeters, that leads to a problem with a wide range of Knudsen numbers (0.001 to 1 or more).

For micron and submicron sizes of the modeled system the mathematical model of gas flow can't be completely formulated within the macroscopic approach. The Navier-Stokes equations with special boundary conditions on walls or the Boltzmann equations in some approximation are usually used in such situation for description of the flow. Both methods have the advantages and the disadvantages. The solution based on the Navier-Stokes equations allows to reduce significantly computing expenses, however Knudsen number within this approach can't be more than 0.1. The solution based on the Boltzmann equation is more expensive; however the Knudsen numbers range is not limited from above. From below this range is limited to values of an order 0.01 in case of which the computational procedure on the basis of Boltzmann equation becomes unacceptable in terms of time costs.

In this paper in the range of Knudsen numbers less than 1 the system of quasigasdynamic (QGD) [1] equations is used; this system is more stable to numerical perturbations in comparison with Navier-Stokes system. The QGD equations need to be corrected and added be the boundary conditions, that is

carried out using the method of molecular dynamics (MD) [2]. For Knudsen numbers of an order unity a direct molecular dynamic simulation is used. As a result, the combination of QGD equations and MD approaches covers the entire range of Knudsen numbers and allows to calculate the gasdynamic processes in systems of real microgeometry at necessary level of detailing.

The paper presents a computational technology on the use of multiscale approach combining the macroscopic description of multicomponent gas flows based the system of QGD equations and the MD models at the microlevel. Combining the models of different levels is carried out by using the method of splitting into physical processes [3]. MD acts as means of subgrid numerical correction of the flow macroparameters. This correction is applied: a) in the Knudsen layer near the channel walls, b) in the gas flow for specification of its equations of state, c) for calculating the gas kinetic coefficients and the exchange terms considering redistribution of momentum and energies between the gas mixture components.

2. Problem statement

At macroscale the system of QGD equations [1] in relaxation approximation is used. At microscale the Newton's equations [2] of classical mechanics describing the motion of separate particles and their interactions are used. It is necessary to consider the interactions: 1) the gas molecules with each other (creating the equations of state of gas mixture, implementing the mixing of components and defining the kinetic coefficients), 2) the gas molecules and the solid surface atoms (describing the boundary-layer phenomena).

The problem of binary gas mixture flow through a metal microchannel is considered as an example of applying the multiscale approach. Figure 1 shows the model geometry of the problem (a two-dimensional view of the average area). The computation of gas flow parameters in the microchannel is a research aim.

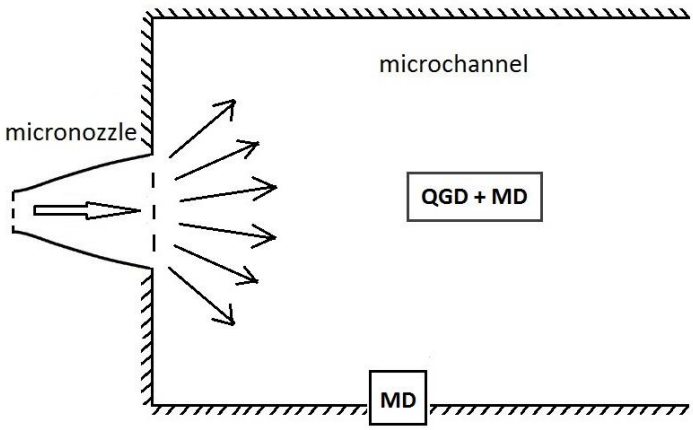

Figure1. The geometry of a model problem for the convenience provided in the form of a two-dimensional view.

Gas is supplied into the microchannel through a micronozzle at the left. At microchannel boundaries instead of usual boundary conditions the values of mass, momentum and energy fluxes calculated by the MD method are used. At the initial moment the gas medium state corresponds to an thermodynamic equilibrium state. In the central part of the microchannel (far from the walls) the simulation is performed at two scale levels (QGD and MD).

2.1. Macromodel

In the case of a gas mixture, the QGD system is written for each gas separately and has an identical form [1]; the equations include exchange terms for the momentum and the energy which are

responsible for the coordination of the mixture parameters. Let us write down this system for a binary gas mixture in a form invariant under the coordinate system, together with the equations of state:

$$\frac{\partial \rho_l}{\partial t} + div\,\mathbf{W}_l^{(\rho)} = 0,\ \ l = a,b, \tag{1}$$

$$\frac{\partial}{\partial t}\rho_l u_{l,k} + div\,\mathbf{W}_l^{(\rho u_k)} = S_l^{(\rho u_k)},\ \ l = a,b,\ \ k = x,y,z, \tag{2}$$

$$\frac{\partial}{\partial t}E_l + div\,\mathbf{W}_l^{(E)} = S_l^{(E)},\ \ l = a,b, \tag{3}$$

$$E_l = \frac{1}{2}\rho_l \left|\mathbf{u}_l\right|^2 + \rho_l \varepsilon_l,\quad P_l = Z_l \rho_l \Re_l T_l,\quad \varepsilon_l = c_{V,l} T_l,\quad l = a,b, \tag{4}$$

where a and b – gases of which mixture consists. Each gas has its own mass density $\rho_l = m_l n_l$, mass m_l, concentration n_l, temperature T_l and macroscopic velocity $\mathbf{u}_l$. Other parameters: P_l – partial pressures, E_l – total energy densities, ε_l – internal energies, Z_l – compressibility factors, $c_{V,l}$ – specific heat capacities at constant volume, $\Re_l = k_B / m_l$ – gas constants (k_B – Boltzmann constant). Vectors $\mathbf{W}_l^{(\rho)}$, $\mathbf{W}_l^{(\rho u_k)}$ and $\mathbf{W}_l^{(E)}$ coincide, up to the sign, with the density fluxes, fluxes of the corresponding components of the momentum density and energy density. They include QGD corrections proportional to Maxwell relaxation time, and depend on the coefficients of viscosity μ_l and thermal conductivity χ_l. The exchange terms $S_l^{(\rho u_k)}$ and $S_l^{(E)}$ take into account the momentum and energy redistribution between the gas mixture components depending on the molecular collision frequency. They contain the components of velocities and energy computed at the molecular level.

The coefficients of viscosity μ_l, thermal conductivity χ_l and compressibility Z_l, and also the specific heat capacities $c_{V,l}$ and other macroparameters for mixture components are determined either from a database of molecular calculations, or by direct MD computations.

The system of QGD equations (1)-(3) is closed by initial and boundary conditions. The initial conditions correspond to an equilibrium state of the gas medium without interactions with external factors. It is possible to consider the case of a quiescent gas medium in the entire computational domain. The densities, velocities, and total energies of the gas components are set at the channel inlet. “Soft” boundary conditions [1] are specified on free surfaces. A special microscopic system consisting of gas molecules and metal atoms is introduced near the channel walls. The boundary conditions on the wall are set as third-kind conditions describing the exchange of mass, momentum components, and energy between the gas mixture in the flow and in the near-wall layer. These conditions involve accommodation coefficients determined by tabulated physical data (which is possible for limited ranges of temperatures and pressures) or computed using the MD method. Another way of formulating the boundary conditions is the direct MD computation of density, momentum, and energy fluxes through the boundary of the near-wall layer.

2.2. Micromodel

In this problem at the microlevel away from the channel walls two types of particles (binary gas mixture) are considered, near the walls the particles constituting the wall material (e.g. metal) are added. The behavior of particles is described by Newton's equations [2]:

$$m_{l,i}\frac{d\mathbf{v}_{l,i}}{dt} = \mathbf{F}_{l,i},\quad \mathbf{v}_{l,i} = \frac{d\mathbf{r}_{l,i}}{dt},\quad i = 1,...,N_l,\quad l = a,b,c, \tag{5}$$

where i – particle index, l – particle kind (a and b – molecules of the first and second gases, c – metal atoms), N_l – total number of particles of kind l. The particle of kind l with index i has its mass $m_{l,i}$, position vector $\mathbf{r}_{l,i}$, velocity vector $\mathbf{v}_{l,i}$ and total force $\mathbf{F}_{l,i}$ acting on this particle.

The interaction between the particles is described by potential functions depending on the particle coordinates. The choice of interaction potential is based on comparing the mechanical properties of computer potential model and real material.

The calculation of the compressibility factor and heat capacity using the MD method is described in detail in [4], the calculation of viscosity and thermal conductivity coefficients of the mixture components using MD is described in [5].

The initial conditions at the microlevel are determined by the equilibrium or quasiequilibrium thermodynamic state of particle system at given temperature, pressure, and mean momentum. The boundary conditions at the molecular level depend on the situation to be simulated. To determine the general properties of the medium, it is sufficient to consider a distinguished three-dimensional volume of it with periodic boundary conditions on all coordinates. In the study of actual geometry microsystems, such as a microchannel, one or several directions are of finite size and shape retention of the object is achieved by the selection of potential or fixing the system. The temperature and total momentum of the system are controlled with the help of thermostats algorithms [6, 7].

3. Computational technology and examples

When solving problems the QGD system of the equations is sampled by the finite volume method [8] on the suitable structured or unstructured grids and is solved on the basis of explicit or implicit schemes on time. MD system of equations is solved by velocity Verlet scheme [9].

Simulation of problems at two scales should be done according to certain rules. It is possible to use MD calculations as directly, combining in one implementation the QGD and the MD, and indirectly, accumulating molecular database calculated earlier and using only a ready base. It is also possible the partial use of MD database and the partial direct MD modeling combined with QGD calculations. Thus, the computational technology assumes 4 types of algorithms.

Algorithms of type 1 include MD calculations of material properties and accumulation of database on these properties. Also, this type of algorithms can be used for full calculations for problems where the characteristic sizes are molecular sizes.

Algorithms of type 2 realize the calculations of gas mixture flows in technical microsystems by means of QGD equations using only the accumulated database. For receiving all necessary value range from the database the method of logarithmic interpolation is used. Conditions of pure gas or gas mixture flows can be very variable, for using this algorithm it is necessary to have access to large memory volumes for database storage and fast use these data by necessity in the calculations. Therefore calculation of MD database for the entire range of possible values can be too expensive in terms of time and information storage.

Algorithms of type 3 produce gas flows in microsystems calculations by means of QGD equations using the molecular database on boundary area and direct MD calculation in a gas flow. The boundary layer includes areas with wall particles; the wall is solid, it has structure and number of solid particles in the volume is many times more than the number of gas particles in the same volume. For this reason computations on boundaries represent one of the most expensive parts of modeling on the necessary memory capacity, operation number, and therefore on time of calculations.

Algorithms of type 4 base on direct macroscopic and microscopic simulations that are being implemented by the method of splitting into physical processes. This method allows to alternate calculations of QGD and MD equations, using MD computation as a subgrid algorithm. Direct MD calculation during computing the problem is most justified if the database on material properties is incomplete or at all is absent. In this case the algorithm of type 4 provides a complete simulation cycle by all necessary data and allows to coordinate processes on micro- and macrolevels, and also to make calculations for a certain specific set of conditions and at the same time to accumulate the database for a case of repeated computing experiments.

Let us describe more detail the algorithm of type 4.

At the microlevel all calculations are made independently in each control volume of a spatial grid, except for boundary cells. In boundary cells the nonlocal MD scheme of computations can be used.

This is especially relevant in a case of large Knudsen numbers (order of 1 and more) when QGD system loses accuracy owing to violation of the gaseous medium continuity hypothesis.

Algorithms of type 4 consist of five basic steps:

1) computing the macroparameters of gas components according to grid analogues of QGD equations excluding exchange terms in grid cells where approximation of continuous medium is valid;

2) MD calculating the exchange terms in average flow field based on local algorithms;

3) return to a macrolevel and correcting the gas momentum and total energy densities;

4) MD calculating the kinetic coefficients, the equations of state parameters and other macroparameters in average flow field, and also the parameters of boundary conditions near the computational domain boundaries and the boundaries between the different medium types;

5) return to a macrolevel and correction of gases moment and total energy densities, and also of a metal surface state.

Criterion for stopping the MD calculations is either the achievement of characteristic time of molecular system evolution (maxwellization time), or small change (for 1-2%) one or more macroparameters of molecular system (average momentum, averages kinetic and/or potential energies).

Presented computational technology allows using the appropriate type of algorithms, depending on the available computing systems and memory capacities. Described multiscale approach allows modeling multicomponent gas flows taking into account the complex geometry of the microchannels, that is provided by means of MD methods. MD calculations determine the kinetic coefficients and exchange terms necessary for computing the system of equations (1)-(3), the compressibility factors and specific heat capacities underlying the equations of state (4), and also boundary conditions.

The technique of numerical modeling is implemented in the form of parallel program tool and is verified on a set of model problems. Subsonic and supersonic flows of pure gases and a binary gas mixture were considered. The obtained calculation results agree with the known tabular data and experimental results. In work [10] the nitrogen and hydrogen mixture flow was calculated on an output from a micronozzle in the semi-open microchannel and further to the free space. The calculation results were close to data of experiments. Also in [10] the combination of the micro- and macromodels of the gas medium in a uniform research object was offered. In [11, 12] interaction of a gas flow with microchannel walls on the example of nitrogen-nickel system was considered. In [5] on an example of the same system the accommodation coefficients were obtained. These calculations represent a technique of obtaining the boundary conditions by direct MD computation. In works [12-15] methods for calculating the thermodynamic equilibrium states in metal-metal, gas-gas and gas-metal systems were developed. In particular, nickel-nickel, aluminum-aluminum, argon-argon, nitrogen-nitrogen, nitrogen-nickel systems were considered. In [4] on the example of nitrogen molecule system the technique of specifying the equations of state was considered. In [5] three methods for determining the kinetic coefficients were presented, comparing methods were produced and examples of calculating the coefficients of nitrogen molecule system were given.

4. Conclusions

For modeling the gases and their mixtures transportation through the microchannels of technical systems the multiscale approach combining the calculations on macro - and microlevels is used. At the macroscale the system of quasigasdynamic equations is used, at the microscale the method of molecular dynamics is used. For the numerical investigation the method of splitting into physical processes is applied (allowing to alternate the calculations at macro- and microlevels). The finite volume method is used for sampling the quasigasdynamic equations on the grids of different types and velocity Verlet scheme is used for implementing the Newtonian equations applied for surface atoms of the microchannel walls and for gas molecules flowing through the channel. The paper presents the computational technology of using the multiscale approach. Four types of technology algorithms are described. A set of the solved model problems is given. The obtained results were compared to experimental data and confirmed a correctness and efficiency of the provided technique.

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